

Ethyl ethylcarbamate
623-78-9 | DTXSID0060775

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 21.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.65e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Methoxy-2-propyl acetate</div> <div>Measured: 2.29</div> <div>Predicted: 7.33</div>	<div>Image not found</div> <div>2-Butoxyethanol</div> <div>Measured: 67.6</div> <div>Predicted: 45.0</div>	<div>Image not found</div> <div>2-(Pyridin-2-yl)ethanol</div> <div>Measured: 28.2</div> <div>Predicted: 35.9</div>
<div>Image not found</div> <div>Hexanoic acid</div> <div>Measured: 28.8</div> <div>Predicted: 31.6</div>	<div>Image not found</div> <div>4-Aminobenzoic acid</div> <div>Measured: 316</div> <div>Predicted: 96.6</div>	